X International Conference on Computational Plasticity
COMPLAS X
E. Oñate and D. R. J. Owen (Eds)

DEVELOPEMENT OF A DISLOCATION-BASED CONSTITUTIVE LAW FOR FCC CRYSTAL ON A WIDE RANGE OF DEFORMATION AMPLITUDE

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Key words: Strain hardening, Dislocations Dynamics, Dislocation-based model

Summary. An original description for crystal plasticity is presented in this work. It is built on a reduced set of constitutive laws whose writing is fully based on physical mechanisms responsible for plasticity in fcc crystal. Dislocation microstructures and their effect on the macroscopic behavior have been studied using 3D Dislocation Dynamics simulations. The result is a model that introduces both isotropic hardening and kinematic hardening without using any phenomenological consideration. Remarkable results are obtained in a wide range of imposed plastic strain amplitude (from small amplitude cyclic loading (10^{-5}) to large strain monotonic loading).

1 INTRODUCTION

Actually, constitutive laws are based on phenomenological approaches. They often fail to predict the behavior of materials when range of deformation amplitude and deformation path is wide, as their identification is closely linked to a particular experimental test. An alternative method consists in establishing physical-based models that include state variables directly linked to the physical mechanisms involved in crystal plasticity (dislocation density, grain size …). If physics of plasticity is well understood and its mathematical transcription is correct, this kind of model will be able to reproduce any loading path and loading amplitude with no fit of parameters.

The model developed in this work exhibits a great ability to predict cyclic or monotonic behavior of fcc crystal. It is based on a physical representation of the dislocation microstructure according to statistical distribution of plastic slip obstacles [1] induced by the microstructure itself (dislocations dipoles in single slip, forest dislocations when multi-slip). This heterogeneous description of the dislocation microstructure leads to a physical description of the kinematic hardening, which represent one of the main lacks of existing dislocation-based model.

A reduced set of equations using a reduced set of parameters (all having a physical meaning) has been written using three-dimensional dislocation dynamics (DD) simulations [1,2]. Comparison of numerical results with experiments has been successfully performed for cyclic and monotonic loadings. An additional study showing the evolution of the stored energy in the microstructure is also presented.

2 CONSTITUTIVE EQUATIONS OF THE MODEL

The aim of the present work is to introduce micro-structural datas in constitutive laws dedicated to plasticity of fcc materials. Following this idea, dislocation microstructures

computed by DD simulations [1,2] have been accurately analyzed. In single slip situations, they show that obstacles to plastic slip are dislocations dipoles, whose height (i.e. strength *s*) are distributed according to an heterogeneous distribution *f*(*s*) that clearly looks like an exponential distribution (standard deviation is equal to mean value $\bar{s}$) (see Figure 1). TEM observations in copper [3] or AISI316L stainless steel [4] confirm this result. The mean strength $\bar{s}$ of obstacles has been identified to the classical hardening law:

$$\bar{s} = \alpha G b \sqrt{\rho} \tag{1}$$

Moreover, we noted that large dislocations loops that accommodate the main part of the imposed plastic strain are periodically stopped by the strength dislocations dipoles rows. This situation induces plastic strain heterogeneity in the vicinity of any obstacle of strength *s*, resulting in a local back stress X_s according to:

$$X_s = GM(\gamma_s - \gamma) \tag{2}$$

where *G* is the shear modulus, *M* is a material coefficient identified with DD simulations, γ_s is the local shear strain around the obstacle of strength *s*, and γ is the crystal shear strain calculated according a weighted sum:

$$\gamma = \int_0^\infty f(s)\,\gamma_s \mathrm{d}s \tag{3}$$

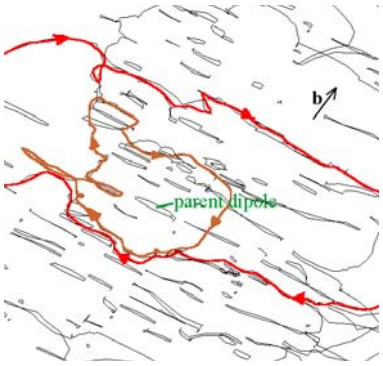

Figure 1: A typical microstructure obtained in a classical situation of single slip is depicted in a thin slice. Many dislocation dipoles act as efficient obstacles to plastic slip, revealed by the pile-up of large dislocations loops.

The flow law [5] governing the local strain rate $\dot{\gamma}_s$ for a given applied resolved shear stress τ is given by:

$$\dot{\gamma}_s = \dot{\gamma}_0 \left| \frac{\tau - X_s}{s} \right|^{1/m} sign(\tau - X_s) \tag{4}$$

meaning that no strain is accommodated provided the local applied stress $\tau - X_s$ becomes slightly greater than the temperature-independent breaking strength *s* of the obstacle. In this expression *m* and $\dot{\gamma}_0$ are respectively a strain rate sensitivity exponent and a reference strain rate.The last law needed to close this set of constitutive equations describes the evolution of the total dislocation density as a function of the strain rate, where *K* is a coefficient linked to the mean free path of a dislocation before being definitively stopped, $\bar{s}$ is the mean resistance of obstacles to plastic slip, P_{stored} is the global power stored by the microstructure, and y_c is the dislocations annihilation distance:

$$\dot{\rho} = \frac{1}{b}\left(\frac{\bar{s}}{\alpha G b K} \cdot sign(P_{stored}) - 2 y_c \rho \right) |\dot{\gamma}| \tag{5}$$

For larger imposed strain or when many slip system are implied, additional DD studies have

been performed. The mathematical formalism remains the same. The only difference results in the use of interaction symmetric matrix between slip systems, whose terms are identified with DD simulations.

3 RESULTS PRESENTATION

The mechanical parameters of metals have been identified thanks to DD simulations [1], in order to fit experimental results [6].

y_c (m)	K	G (GPa)	M	m	γ_0	τ_0 (MPa)	b(Å)	α	λ
$2*10^{-9}$	35	45	2	0.05	10^{-10}	4	2.56	0.3	0.8

Table 1 : Parmeters for pure copper at $T = 295\ K$.

The results for a cyclic loading of a copper crystal in single slip are presented in the Figure 2a. It shows the evolution of the hysteresis loops for imposed plastic shear strain amplitude $\Delta\gamma_p = 3\times10^{-3}$. The evolution of the shape and of the amplitude is in good agreement with experiments [6]. On the beginning of the cycling, there is no effect of kinematic hardening, as the dislocation microstructure is homogeneous. As cycling proceeds, both isotropic and kinematic hardening increases.

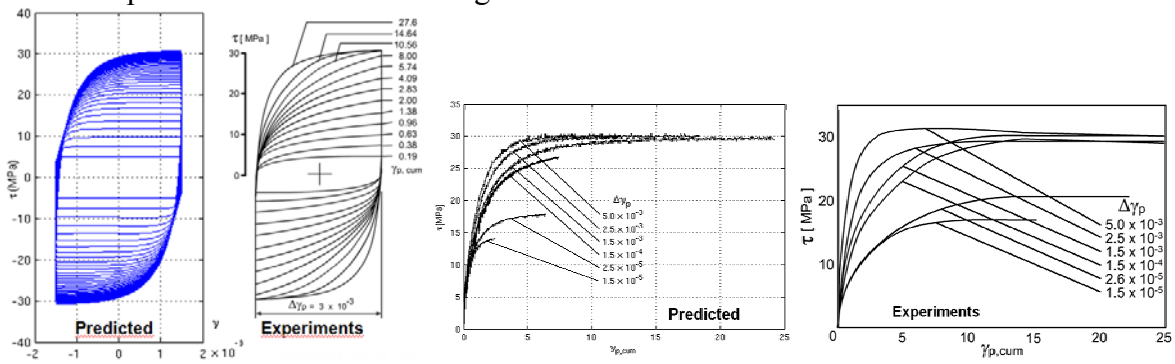

Figure 2: (a) Comparison of the evolution of hysteresis loops during cycling of a single copper crystal. (b)Predicted cyclic hardening curve at different imposed plastic strain and its corresponding experiments.

The Figure 2b is a comparison of the cyclic hardening curves. Once again, it is in good agreement with experimental findings results [6]. The saturation stress is about 30 MPa for any imposed plastic strain between 10^{-4} and 10^{-2}.

In order to get a better understanding of kinematic hardening and its effect, a study of energy balance of the model has been performed. Figure 3a reveals the perfect balance between furnished power, dissipated power, and stored power. It can be seen that during unloading, when the imposed plastic strain rate is reversed, the stored power becomes negative, meaning that the microstructure gives back stress. The evolution of the stored energy has also been plotted in the Figure 3b. It shows that during each cycle, a part of the stored energy is definitively stored, whereas another part is only temporally stored, as it is given back during unloading. A correlation between stored energy and dislocation density has been directly established: $E_{\text{stored}} = \beta G b^2 \rho$.

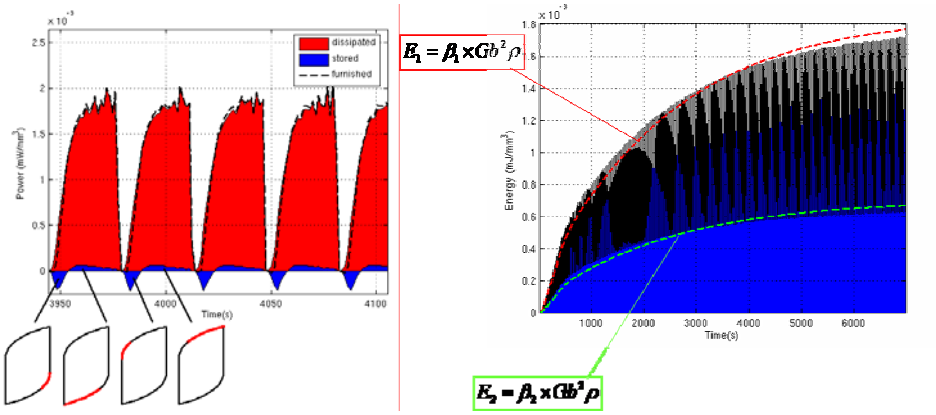

Figure 3: (a) Power evolution as a function of the time during cycling. (b) Energy evolution during cycling.

Figure 4 depicts the results of the same set of constitutive laws for the monotonic loading of a single crystal, for different orientation of loading. Note that no fit of coefficient has been necessary. A good agreement between simulation and experiment is observed.

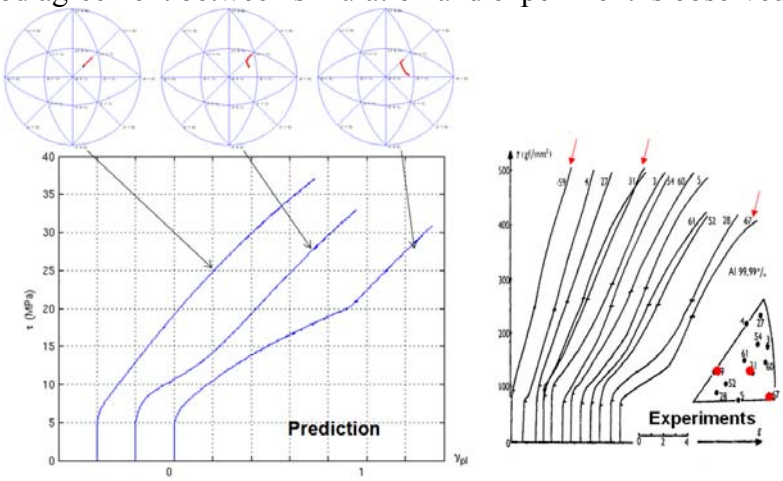

Figure 4: Stress-strain curve for monotonic loading and its corresponding experiments.

4 CONCLUSIONS

The model presented in this work is able to describe typical plastic behaviors of single fcc crystals in a large range of imposed plastic strain amplitude. Its constitutive equations and its associated parameters have been identified according physical studies of dislocation microstructures. It is an original description of plasticity that may substitute to phenomenological descriptions.

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